Endosulfan sulfate

1031-07-8 | DTXSID3037541

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		**Training (75%)**		**Test (25%)**	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 15.6 days

Global applicability domain: Outside

Local applicability domain index: 1.01e-01

Confidence level: 7.00e-01

Nearest Neighbors from the Training Set

Image not found

Squalane
Measured: 5460
Predicted: 49.4

Image not found

Norphytane
Measured: 5460
Predicted: 32.6

Image not found

Tetradeca-1,13-diene
Measured: 367
Predicted: 8.69

Image not found

2,4-Dimethylheptane
Measured: 61.9
Predicted: 4.29